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Modeling and optimizing oxygen transfer in small scale reactors using computational fluid dynamics

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BACKGROUND

The most common way to describe oxygen transfer in bioreactors is via the oxygen transfer coefficient, k_La, which describes the dynamic relationship between the oxygen concentration (C) and the oxygen saturation concentration (C*) assuming a perfectly mixed liquid according to the following equation:

$$\frac{dC}{dt} = k_L a(C^* - C)$$

In computational fluid dynamics (CFD) simulations however, 'k_La' is most often separated into the mass transfer coefficient 'k_L' and the specific interfacial area 'a'. One common way to evaluate k_L is then using the correlation

$$k_L \propto \sqrt{\frac{D_L}{\nu}}(\varepsilon\nu)^{0.25}$$

which relates it to the diffusion coefficient (D_L) of oxygen, the viscosity (ν) and the energy dissipation (ε) in the fluid.

METHOD

Experimental k_La and mixing times values for a 1 ml impeller driven microbioreactor [1] were simulated using the computational fluid dynamics software ANSYS CFX 14.0. The simulations were performed on a two-phase system (water and air) using a k -ε turbulence model.

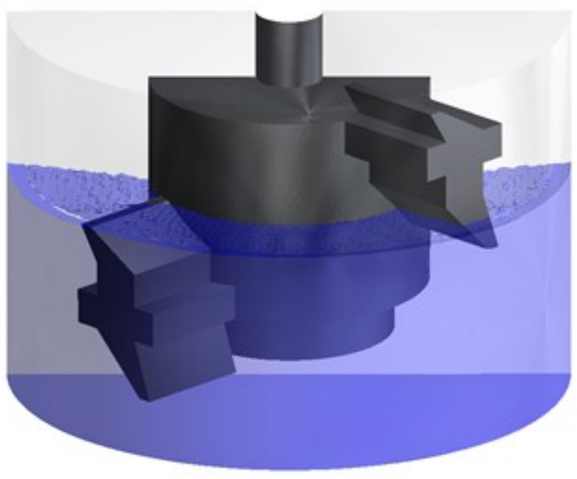

Figure 1. The two-phase system showing the water, air, and the geometry of half of the microbioreactor

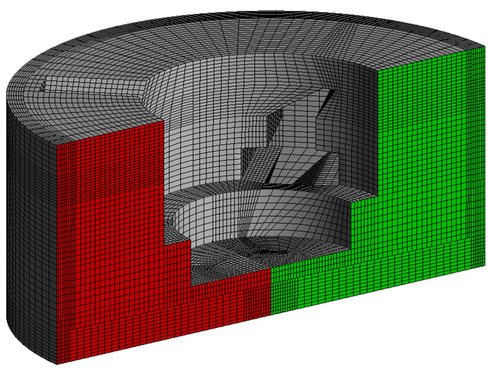

Figure 2. One of the computational meshes used for the simulations. Rotational periodicity was applied between the red and the green surface

RESULTS AND DISCUSSION

STEADY STATE OXYGEN TRANSFER SIMULATIONS

Steady state simulations were performed where the integrated energy dissipation term ε in the liquids as well as the mass flows through the rotational periodicity in Figure 2 were calculated. The experimental values for k_La, the simulated values of $\varepsilon^{0.25}$, and the mass flows are scaled and plotted in Figure 3. As it can be seen they all follow the same trend once correlated with a constant. It is therefore questionable if it is reasonable to use the very model dependent factor $\varepsilon^{0.25}$ once modeling the oxygen transfer, or if other options (e.g. the mixing time) are better.

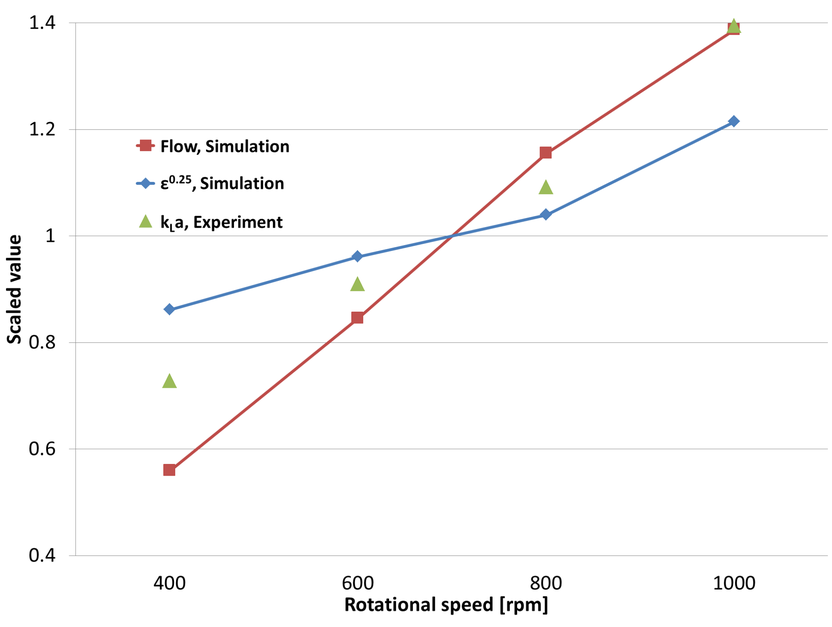

Figure 3. Scaled values for the simulated $\varepsilon^{0.25}$, the simulated mass flow and the experimental k_La value for 400, 600, 800 and 1000 rotations per minute (rpm)

RESULTS AND DISCUSSION

MIXING SIMULATIONS

The steady state results for the volume fractions and fluid velocities were used in transient simulations where the behavior of an additional variable, representing a color dye, was investigated over time. The additional variable was added to the system from the source point shown in Figure 4b and allowed to spread in the domain until reaching the final concentration c_{final}. The mixing time was then evaluated as when the global mixing quality (MQ_{global}) had reached either 75% or 90%. Figure 5 shows that the simulations follow the experimental data well.

$$MQ_{local} = 1 - \left|\frac{c_{final} - c(t, position)}{c_{final}}\right|$$

$$MQ_{global}(t) = \frac{\iiint_V MQ_{local}\, dV}{V}$$

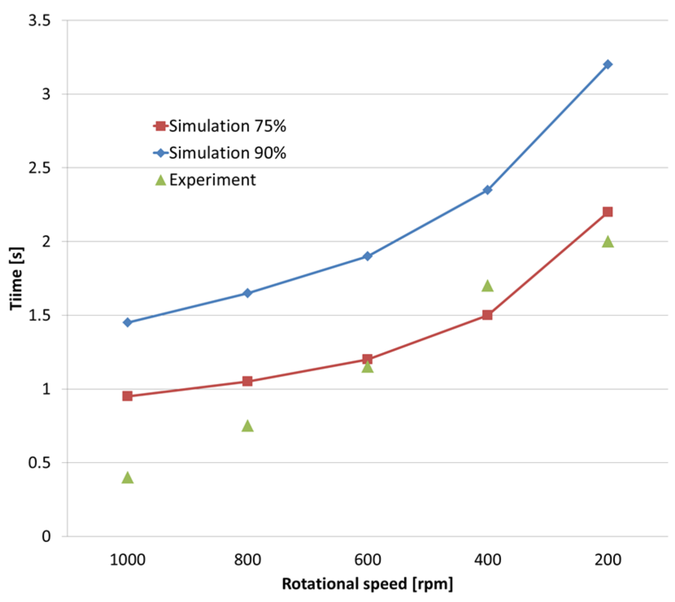

Figure 5. The simulated mixing times compared to experimental values

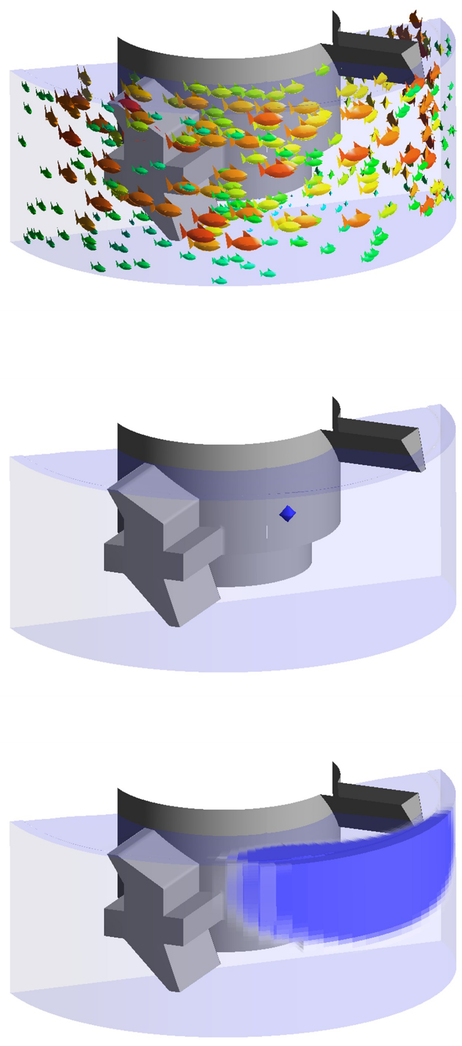

Figure 4. The velocity vectors represented as fishes (a), the position of the source point (b), and the spread fo the dye in the reactor (c)

OXYGEN TRANSFER SIMULATIONS

The water and air were both set to be variable composition mixtures of oxygenated water and non-oxygenated water and gaseous O_2 and N_2 respectively. The already available interfacial equilibrium model 'Henrys Law' was then applied and transient simulations were performed starting with a low and homogenous concentration of oxygenated water in the liquid phase. As presented in Figure 6, the oxygenated water is as expected more evenly distributed for 1000 rpm than for 200 rpm. The higher concentration of oxygenated water at the surface for the 200 rpm case is believed to illustrate the importance of mixing in order to improve the oxygen transfer.

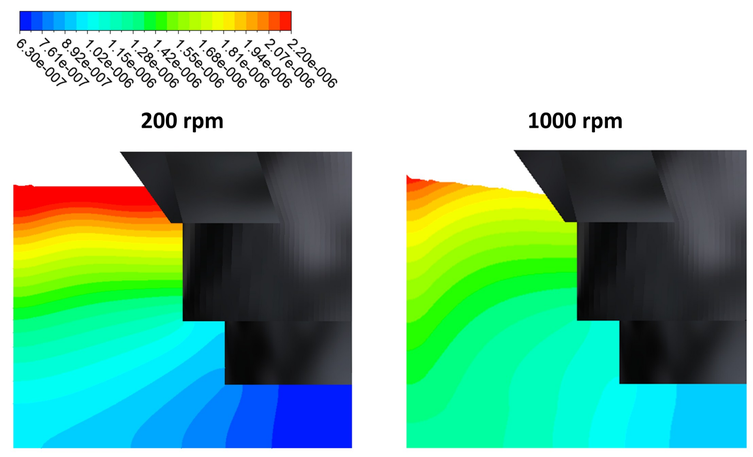

Figure 6. The mass fraction of oxygenated water in the liquid phase after 5 s for 200 rpm and 1000 rpm

FUTURE WORK AND PERSPECTIVE

The oxygen transfer model will be improved with the intention to capture the differences between the varying rotational speeds even better. The influence on the overall oxygen transfer from the separate parameters surface area, mixing, and oxygen gradient over the interphase will also be investigated.

An optimization algorithm will be developed where the 3D shape of the reactor can be varied and optimized with respect to its oxygen transfer characteristics. The design performing best in the simulations will subsequently be fabricated and evaluated experimentally in the lab with on-line oxygen measurements.

ACKNOWLEDGEMENTS: This PhD project is founded by Novo Nordisk Foundation

REFERENCE: 1. Bolić, A., Krühne, U., Prior, R. A., Vilby, T., Hugelier, S., Lantz, A. E., Gernaey, K. V., 2012. One-Millilitre Microbioreactor with Impeller for Improved Mixing, Poster session presented at 12th International Conference on Microreaction Technology (IMRET12), Lyon, France.

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